Dirac Hartree-Fock for Finite Nuclei Employing Realistic Forces

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Abstract

We discuss two different approximation schemes for the self-consistent solution of the *relativistic* Brueckner-Hartree-Fock equation for finite nuclei. In the first scheme, the Dirac effects are deduced from corresponding nuclear matter calculations, whereas in the second approach the local-density approximation is used to account for the effects of correlations. The results obtained by the two methods are very similar. Employing a realistic one-boson-exchange potential (Bonn A), the predictions for energies and radii of ^{16}O and ^{40}Ca come out in substantially better agreement with experiment as compared to non-relativistic approaches. As a by-product of our study, it turns out that the Fock exchange-terms, ignored in a previous investigation, are not negligible.

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One of the most fundamental challenges of nuclear many-body theory is to derive the bulk properties of nuclei, like energies and radii, from a realistic nucleon-nucleon (NN) interaction. Here, the term "realistic" refers to nuclear potentials which reproduce the two-nucleon data accurately. Representative examples are the Paris NN potential [1] and the models developed by the Bonn group [2]. Typically, these forces contain strong components of short range, which make it inevitable to carefully account for the two-nucleon correlations at short inter-nucleonic distances. In the Brueckner-Hartree-Fock (BHF) method this is done by solving the Bethe-Goldstone equation. The resulting G-matrix can be understood as an effective interaction which incorporates effects of NN correlations and depends on the properties of the nuclear system under investigation.

For many years, calculations of this kind have been performed with only limited success. More than 20 years ago, Coester *et al.* [3] observed that, in an energy *versus* density plot, the saturation points of nuclear matter as obtained in BHF calculations employing different realistic potentials are located along a band ('Coester band') that does not include the empirical value. For example, one may find a realistic NN interaction which reproduces the binding energy of nuclear matter correctly, but at a saturation density which is about twice the empirical one. *Vice versa*, a different realistic interaction may predict the saturation density correctly but yield a binding energy of about 11 MeV per nucleon rather than the empirical 16 MeV.

In the past, there have been many attempts to improve nuclear many-body theory within the framework of non-relativistic quantum mechanics. Three-nucleon correlations and other corrections to BHF have been considered, however, without substantial success [4]. A phenomenon similar to the Coester band for nuclear matter, has been found for finite nuclei [5, 6, 7]: BHF calculations yield either correct binding energies but too small radii, or correct radii but too small binding energies. We mention that Kuo *et al.* [8] were able to improve the predictions for nuclear matter by including effects of so-called particle-particle/hole-hole ring diagrams (long-range correlations). However, it appears that this method does not improve the predictions for finite nuclei, sufficiently [9].

Motivated by the success of the σ - ω model of Walecka and Serot [10], attempts have been made to incorporate the relativistic features of this approach also in nuclear structure calculations which are based upon the realistic NN force. Such Dirac BHF (DBHF) calculations, as this has become known, have been performed for nuclear matter by, e. g., Shakin and collaborators [11], Brockmann and Machleidt [12], and ter Haar and Malfliet [13]. The basic aspects of this approach have been thoroughly investigated by Horowitz and Serot [14]. In the DBHF approach,

one accounts for the fact that the relativistic nucleon self-energy in nuclear matter is given essentially by a large attractive scalar ('σ') and repulsive vector ('ω') field. The single-particle motion is described by a Dirac equation which includes this self-energy. Due to the scalar field, the nucleon mass is reduced enhancing the ratio between small and large components of the Dirac spinors. Moreover, the sigma field decouples causing a strongly density-dependent repulsive effect.

Due to these features, Brockmann and Machleidt [12, 15] were able to reproduce nuclear matter saturation correctly in a DBHF calculation employing a realistic one-boson-exchange NN potential ('Bonn A'). Now, the crucial question is whether the DBHF approach can also explain the bulk properties of finite nuclei.

The self-consistent solution of the DBHF equation for finite nuclei is much more involved than for nuclear matter. Therefore, two different approximation schemes have been developed. In the first scheme [16], the pair correlations are calculated in the finite nucleus under consideration whereas the medium dependence of the Dirac spinors is taken into account via the local-density approximation. Thus, the Bethe-Goldstone equation is solved directly for the finite nucleus satisfying the self-consistency requirement of conventional BHF. Relativistic medium effects are taken into account by evaluating the potential matrix elements and the kinetic energy in terms of in-medium Dirac spinors.

In Table 1 (column DBHF), we show results of relativistic BHF calculations performed according to scheme one for the nuclei ^{16}O and ^{40}Ca. In all calculations of this note, the Bonn A potential [2] is applied. It is interesting to compare these results with non-relativistic BHF calculations, in which the medium-dependence of the Dirac spinors is ingnored (column BHF of Table 1). It is seen that the Dirac effects increase the binding energy *and* the charge radius. Thus, the DBHF results are in better agreement with experiment. Typically, the remaining discrepancy between the DBHF results and experiment is only about one half of the corresponding discrepancy in conventional BHF calculations. For ^{16}O, results have been reported in Ref. [16]. They are confirmed by our present investigations, which also includes ^{40}Ca.

In the second approximation scheme, one treats the pair correlations in local-density approximation, while the Dirac equation is solved directly for the finite nucleus. This can be done by defining an effective medium-dependent meson-exchange interaction based upon the nuclear matter G-matrix. Since the G-matrix is density-dependent, so are the coupling constants of the effective interaction which are adjusted such as to reproduce the G-matrix [17, 18]. A simple and successful calculation along this line has recently been reported by Brockmann and Toki [19]. For the

effective interaction, they consider σ and ω exchange, adjusting the coupling constants such that a simple Dirac-Hartree calculation reproduces the nuclear matter DBHF results. The density-dependence of the resulting coupling constants is displayed in Fig. 1. The coupling constants for both σ and ω decrease with increasing density. This is clearly the correlation effect [18].

Employing these density-dependent coupling constants in a Dirac-Hartree calculation for finite nuclei, one obtains good agreement between theory and experiment (see Ref. [19] and column RDH in our Table 1), keeping in mind that these are parameter-free calculations based upon a realistic NN interaction. Our RDH results, displayed in Table 1, deviate slightly from those obtained by Brockmann and Toki [19]. The differences can be understood as follows: First, we include a center-of-mass correction (as discussed, e. g., in Ref. [16]) to allow for a comparison between the various approximations displayed in Table 1. Secondly, we observed a sensitivity of the results on the extrapolation of the coupling constants to densities below the lowest density considered by Brockmann and Toki. We tried to remove this sensitivity by inspection of nuclear matter at low densities. The Dirac-Hartree, as well as the Dirac-Hartree-Fock equation discussed below, were solved by a matrix diagonalisation method, expanding the wavefunctions in a basis of states for a spherical cavity [20]. The new computer code has been tested by comparing the results with those presented by Bouyssy *et al.* [21].

Inspection of Table 1 reveals that there are significant differences between the RDH and DBHF results. Since both schemes are approximations to a complete self-consistent calculation for a finite nucleus, at least one approach must be a poor approximation.

The natural step beyond the relativistic density-dependent Hartree (RDH) approximation is relativistic Hartree-Fock. Assuming a σ - ω model with density dependent coupling constants g_σ and g_ω, the scalar part of the nucleon self-energy in nuclear matter at density ρ can be written as [10, 18]

$$\begin{aligned} U^s(k,\rho) &= \frac{-4}{(2\pi)^3}\frac{g_\sigma^2(\rho)}{m_\sigma^2}\int_0^{k_F} d^3q \frac{M^*(q,\rho)}{E^*(q,\rho)} \\ &\quad + \frac{1}{4\pi^2 k}\int_0^{k_F} q\,dq \frac{M^*(q,\rho)}{E^*(q,\rho)}[\frac{1}{4}g_\sigma^2(\rho)\Theta_\sigma(k,q) - g_\omega^2(\rho)\Theta_\omega(k,q)] \end{aligned} \quad (1)$$

using the notation of Serot and Walecka (Ref. [10], pp. 130-131) The first line in this equation is the Hartree contribution and the second line the Fock term. At each density, we adjust the coupling constants g_σ and g_ω such that the scalar part of the self-energy and the total energy per nucleon as obtained in the DBHF calculation for nuclear matter are reproduced by a Hartree-Fock calculation using this simple

σ - ω model. The resulting coupling constants are reduced as compared to the Hartree analysis, see Fig. 1. This can easily be understood by comparing Eq. (1) and the corresponding expression for the vector component for the self-energy with the expressions of the Hartree scheme. Notice that the density dependence is very similar in both cases.

The density-dependent coupling constants deduced in the Hartree-Fock analysis of the DBHF nuclear matter results can be employed in a Dirac-Hartree-Fock calculation for finite nuclei. Comparing the results of this relativistic, density-dependent Hartree-Fock (RDHF) scheme with those obtained in the RDH approximation (see Table 1) one observes that the Fock terms reduce the binding energies and charge radii. Thus, the very good agreement of the RDH results with experiment was just fortuitous and is lost when the Fock terms are included.

There is, however, good agreement between the DBHF and RDHF results for ^{16}O. For ^{40}Ca, this agreement appears less close. However, one has to keep in mind that it requires only a slight modification in the NN interaction to reduce the energy and increase the radius, i. e., to "move" the results parallel to the Coester band, whereas it is very difficult to achieve a modification perpendicular to the Coester band. In this sense, energies and radii calculated in DBHF and RDHF are very close. This implies that both schemes, treating either the Dirac effects or the effects of correlations in a local density approximation, yield very similar results *if the Fock effects are included*. This can be interpreted as an indication that DBHF and RDHF are reliable approximations for a self-consistent relativistic BHF calculation for energies and radii of finite nuclei. In order to close the gap between the results obtained in DBHF (and RDHF) and experiment it may be necessary to consider three-nucleon correlations or other improvements of the many-body approach beyond relativistic BHF. Details in the spectrum of single-particle energies of RDHF should be improved by taking additional mesons in the parameterization of the effective NN interaction into account [18].

In summary, we have calculated the groundstate properties of ^{16}O and ^{40}Ca using two different approximation methods for solving the relativistic Brueckner-Hartree-Fock equations. The predictions, which are very similar for both approximations, are in substantially better agreement with experiment as compared to conventional, non-relativistic calculations. Fock terms must not be neglected. Remaining small, but distinct discrepancies between theory and experiment represent a challenge for future research in nuclear many-body theory.

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Fig.1: Density-dependent coupling constants deduced from the Hartree and Hartree-Fock analysis of the DBHF results for nuclear matter using the Bonn A potential [2]. The upper part of this figure displays the meson-nucleon coupling constant for the scalar meson (with m_σ=550 MeV), while the lower half shows the result for the vector meson (with m_ω= 783 MeV).

Table 1. Ground-state properties of ^{16}O and ^{40}Ca. The total energy per nucleon (E/A), the charge radius (r_c), and the proton single-particle energies (ϵ_i) as predicted by non-relativistic Brueckner-Hartree-Fock (BHF), relativistic Dirac-BHF of Ref. [16] (DBHF), relativistic, density-dependent Hartree (RDH), and relativistic, density-dependent Hartree-Fock (RDHF) calculations are compared to experiment (last column). In all calculations the Bonn A potential [2] is used.

	^{16}O				
	BHF	DBHF	RDH	RDHF	Exp
E/A [MeV]	-5.95	-7.56	-7.79	-7.36	-7.98
r [fm]	2.31	2.46	2.67	2.47	2.70
$\epsilon_{s1/2}$ [MeV]	-56.6	-49.8	-43.1	-44.7	-40±8
$\epsilon_{p3/2}$ [MeV]	-25.7	-23.0	-22.3	-23.8	-18.4
$\epsilon_{p1/2}$ [MeV]	-17.4	-13.2	-17.5	-15.8	-12.1
	^{40}Ca				
	BHF	DBHF	RDH	RDHF	Exp
E/A [MeV]	-8.29	-8.64	-8.20	-7.93	-8.5
r [fm]	2.64	3.05	3.35	3.13	3.50
$\epsilon_{d5/2}$ [MeV]	-30.2	-21.9	-19.8	-21.2	-14±2
$\epsilon_{1s1/2}$[MeV]	-24.5	-13.8	-15.4	-14.2	-10±1
$\epsilon_{d3/2}$ [MeV]	-16.5	-10.2	-14.5	-13.2	-7±1